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Broer, W.; Hoenders, B. J.

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Natural modes and resonances in a dispersive stratified N -layer medium

W Broer and B J Hoenders

University of Groningen, Centre for Theoretical Physics and Zernike Institute for Advanced Materials, Nijenborgh 4, NL-9747 AG Groningen, The Netherlands

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Abstract

The properties of the natural modes in a dispersive stratified N -layer medium are investigated. The focus is on the (over)completeness properties of these modes. Also the distribution of the natural frequencies is considered. Both the degree of (over)completeness and the natural frequency distribution turn out to be totally different from what is known for the non-dispersive case.

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1. Introduction

Natural modes arise in connection with the scattering of an incoming wave on an object. In this context, they are defined as those solutions of the scattering operator which exist in the whole three-dimensional space \mathbb{R}^3 , satisfy the boundary conditions at the surface of the finite scatterer, and represent outgoing waves outside the medium. Natural modes were first discovered by Cauchy in 1827 [1], and then later applied by Thomson [2], Kolářček [3], and Abraham [4] to various scattering problems. For a non-dispersive medium they are known to have the following properties [5–7]:

- (a) They are complete within the open domain, but not always up to the boundary. (Think of Gibbs' phenomenon of a Fourier series, not necessarily representing the approximated function at the endpoints.)
- (b) Mathematically they are 'double' complete, there are two complete sets of natural modes.
- (c) The complex eigenvalues k_n satisfy $k_n = -k_n^*$.

In this paper, completeness of the natural modes is understood to mean that the solution of the governing partial differential equation, subject to the boundary conditions set by the physical system, can be written as a linear combination of the natural mode eigenfunctions, i.e. this solution and the linear combination of eigenfunctions are 'arbitrarily close' to each other. As these eigenfunctions satisfy the same partial differential equation, they are a subset of L^2_{loc} and hence the definition of completeness given in appendix A.3 also applies to them.

An example from quantum mechanics [8] can give a general idea of the concepts involved. From the time-independent Schrödinger equation

$$(\nabla^2 + k^2)\psi(\vec{r}) = U(\vec{r})\psi(\vec{r}) \quad (1)$$

and the Green's function associated with it

$$G(\vec{r}, \vec{r}'; k) = \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \quad (2)$$

we derive the corresponding scattering integral equation

$$\psi(\vec{r}) = \psi^{(i)}(\vec{r}) - \frac{1}{4\pi} \int_V \psi(\vec{r}') U(\vec{r}') G(\vec{r}, \vec{r}'; k) d^3r'. \quad (3)$$

It is of fundamental importance to note that this integral equation is *not* the standard Fredholm integral equation of the second kind because of the *nonlinear* dependence of the kernel on k . Therefore, the natural modes are a generalization of the results of classical Fredholm theory: they are the solutions of the homogeneous integral equation in terms of which it is to be expected that the solution of the scattering integral equation can be written inside the domain of the scatterer.

Mathematically, natural mode eigenfrequencies are complex eigenvalues of a linear or linearized differential equation, subject to certain non-classical Sturm–Liouville boundary conditions, see [9–14]. In optics (if this differential equation is the wave equation), these eigenfrequencies correspond to the singularities of the system, i.e. the singularities of the scattering matrix [15]. Physically, the natural mode formalism is a tool to describe the *energy dissipation* of a system. The imaginary parts of the eigenvalues indicate the amount of the energy loss of the system. (Similar to a harmonic oscillator with damping; the imaginary part of the frequency equals the damping coefficient.) As such it is used in various fields of physics, ranging from classical wave mechanics, computational biophysics and mathematical physics to general relativity and quantum gravity. (See, e.g. [16, 17] for applications in general relativity.)

In the context of photonic crystals a (complex) natural mode frequency can be related to the *transmission spectrum* of the medium: the real part of the frequency indicates the position of a resonance peak, and its imaginary part corresponds to the full width at half maximum of the peak. In other words: if the wavelength is chosen to correspond to the real part of the natural mode frequency, then the photonic crystal will transmit more electromagnetic radiation than otherwise.

Another important property of natural modes in general is that they *can exist in the medium without the presence of an incoming or driving field* ψ_{inc} . This can be understood in terms of internal (electron) oscillations of the scatterer: those oscillations will continue even after the driving field is long gone.

This paper is organized as follows: the following section concerns the calculation of natural mode frequencies in the physically important special case of (non-dispersive) photonic band gap (PBG) media. The third section covers similar calculations for dispersive stratified N -layer (SNL) media: it is shown that the natural mode frequencies cluster near the resonances in the Lorentz model. The fourth section addresses the question whether the natural mode eigenfunctions can describe the actual electromagnetic field in a dispersive (SNL) medium, (i.e. whether they are complete according to the definition given in appendix A.3), and whether such a representation is unique (i.e. whether they are ‘overcomplete’). Some concluding remarks are made in the final section.

2. Natural mode frequencies and non-dispersive N -layer media

The goal of this section is to find natural mode eigenfrequencies of stratified non-dispersive n -layer media whose respective refractive indices are assumed to be constant. These eigenfrequencies can be defined as the singularities in the transmission and reflection coefficient of the system. (see, for instance [5] and [15]) which both therefore, as we know, have the same denominators.

Generally, for a system of two layers or more, the natural mode frequencies cannot be found exactly. They satisfy a transcendental equation, which can be solved numerically or for ‘large’ values (for more details, see appendix A.1).

However, if we limit ourselves to the case of normal incidence (so there is no angular dependence), and TE transmissions in a periodic medium, we can find the resonance frequencies exactly in, for instance, a system of four periods. Each period consists of two layers each with refractive indices n_1 and n_2 , respectively. Another restriction we would like to make is the following: the thicknesses of the two layers d_1 and d_2 , respectively, are chosen in such a way that

$$n_1 d_1 = n_2 d_2 = \frac{\lambda_{\text{ref}}}{4}, \quad (4)$$

for a certain λ_{ref} . As is well known, this particular choice, which defines the class of so-called quarter-wave stacks, simplifies to a great extent the analysis of the system at hand, [18]. We remark in passing that these systems are optimized for reflection of pulses with center λ_{ref} , because the reflected waves from each layer are all exactly in phase at this wavelength. Such a medium can be used to create planar dielectric waveguides, for instance. For more details we refer to [19].

According to Wolter [18], for the case of TE illumination, the numerator (Z_m) and the denominator (N_m) of the reflection coefficient for a 2D stratified N -layer system may be found by means of the following recursive relations¹:

$$Z_m = (g_m - g_{m-1}) e^{-i\delta_{m-1}} N_{m-1} + (g_m + g_{m-1}) e^{i\delta_{m-1}} Z_{m-1} \quad (5a)$$

$$N_m = (g_m + g_{m-1}) e^{-i\delta_{m-1}} N_{m-1} + (g_m - g_{m-1}) e^{i\delta_{m-1}} Z_{m-1} \quad (5b)$$

$$Z_1 = g_1 - g_0, \quad N_1 = g_1 + g_0, \quad (5c)$$

where m represents the number of interfaces (see, figure 1) and the following shorthand notations are used:

$$g_m := \frac{n_m \cos \theta_m}{\mu_m}, \quad \delta_m := \frac{n_m d_m \omega \cos \theta_m}{c}. \quad (6)$$

These formulae apply to a general 2D stratified N -layer system. Note that we use a different sign convention from the one Wolter used: we assume a time dependence of $e^{-i\omega t}$, whereas he chooses one of $e^{i\omega t}$. Wolter’s recursion formula follows from the requirement that the fields and their derivatives must be continuous at the interfaces. Then, for a single layer ($m = 2$, see figure 1) it follows that we have:

$$Z_2 = (g_2 - g_1)(g_1 + g_0) e^{-i\delta_1} + (g_2 + g_1)(g_1 - g_0) e^{i\delta_1} \quad (7a)$$

$$N_2 = (g_2 + g_1)(g_1 + g_0) e^{-i\delta_1} + (g_2 - g_1)(g_1 - g_0) e^{i\delta_1}. \quad (7b)$$

The frequencies of the natural modes are the zeros of (7b). This equation can be solved exactly, but this is no longer possible in the case of two- and more layers, (for more details, see appendix A.1).

¹ The numerator of the *transmission* coefficient of a system with m interfaces is $2^m \prod_{i=1}^m g_i$, and as noted its denominator is identical to that of the reflection coefficient.

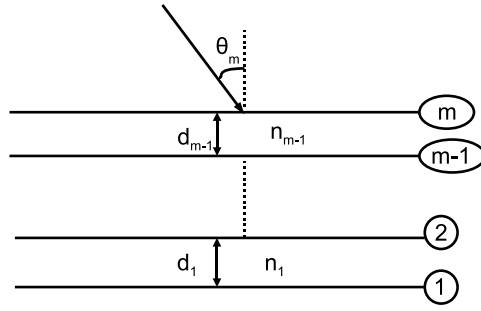


Figure 1. Sketch of the parameters and geometry of the problem. There are m interfaces and $m - 1$ slabs. As we assume normal incidence ($\theta_m = 0$) there is no angular dependence.

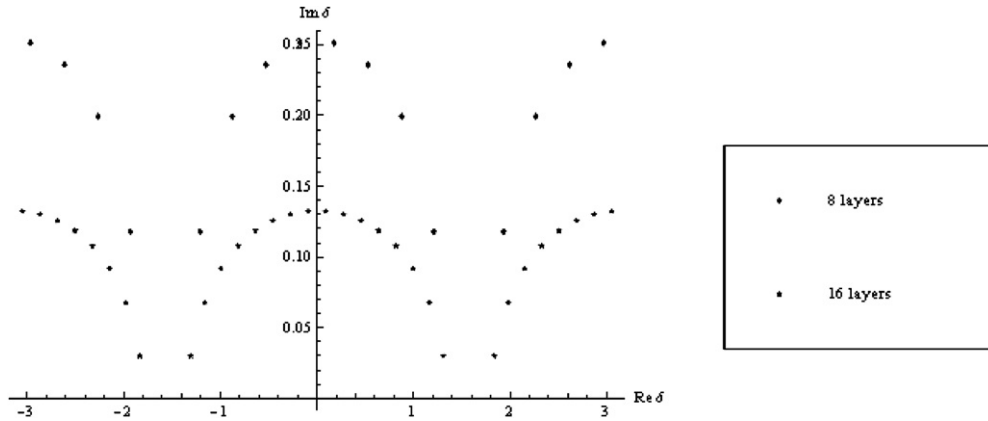


Figure 2. Natural mode frequencies of two non-dispersive, 1D SNL media quarter-wave stacks. The polygons represent the mode frequencies of an eight-layer system and the asterisks represent those of a 16-layer system. The ratio between the refractive indices of the two layers is $\frac{n_1}{n_0} = 1.5$ in both cases.

In the particular case of normal incidence we have $\cos \theta_m = 1$ for all integers m . Also there are only two possible values of n_m and only one possible value of $n_m d_m$. As a consequence, there are only two possible values for g_m ($\mu_m = 1$ for all integer m) and only one variable δ . We will restrict ourselves to non-magnetic media, namely $\mu_m = 1$.

As Settini *et al* [20] noted, under these (restrictive) conditions natural mode frequencies of N -layer media can be found exactly. The natural frequencies of an eight- and a 16-layer system are plotted in the complex plane in figures 2 and 3.

Something similar applies to the TM case; only the following definition needs to be changed with respect to the TE case:

$$g_m := \frac{\mu_m \cos \theta_m}{n_m}. \quad (8)$$

Because we chose this medium to be non-dispersive the refractive indices are constant, so only the values of the parameters change, not the actual pattern of the mode frequencies. (It is useful to remember that Settini and Wolter use different conventions regarding the time dependence of the oscillations, just like in the previous case.)

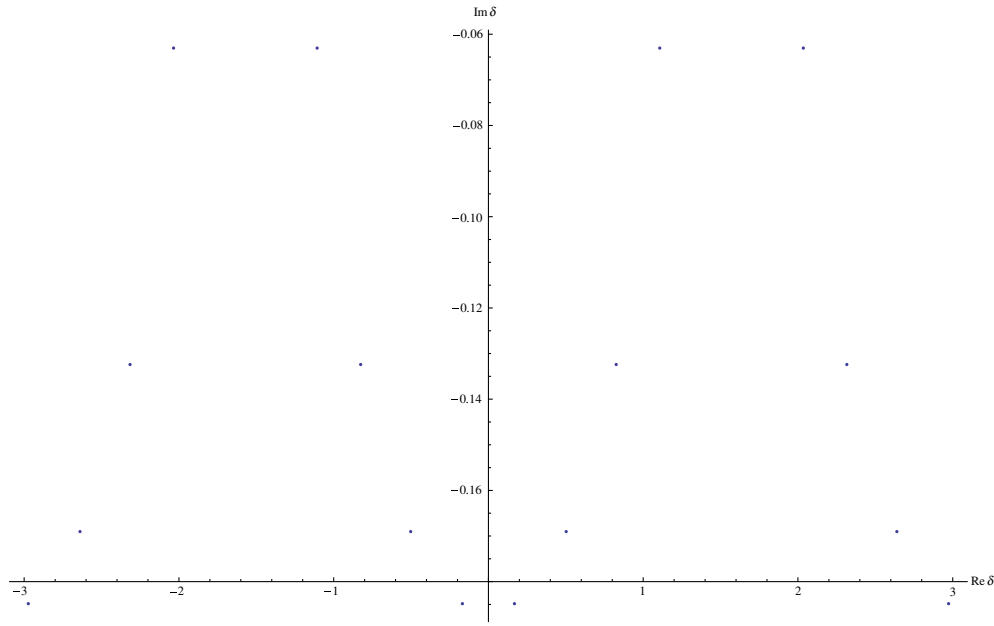


Figure 3. Natural mode frequencies of a non-dispersive, 1D SNL medium with four quarter-wave stacks. The ratio between the refractive indices is in this case $\frac{n_1}{n_0} = 2$.

As we noted before, the real part of a natural mode frequency corresponds to the position of a resonance peak in the transmission spectrum; its imaginary part is related to the broadness (the full width at half maximum) of the peak. The eigenfrequency distributions shown in figure 2 leads to the observations that the number of peaks within an interval $0 \leq \text{Re}(\delta) \leq \pi$ increases proportionally to the number of layers (a system of N layers leads to a polynomial of degree N in $e^{i\delta}$). Also, the peaks become narrower (the imaginary parts of the natural mode frequencies are lower) in a system of 16 layers than in a system of eight layers. However, the position of the ‘gap’ (i.e. interval in the spectrum without peaks) does not change. Increasing the ratio between the two refractive indices results in lower (absolute values of) imaginary parts of the mode frequencies, so resonance peaks in the transmission spectrum become narrower. These results were found in [20] and confirmed by (5).

3. Calculation of natural mode frequencies in dispersive media

In this section we shall investigate the consequences of allowing the medium to be temporally dispersive. The refractive index of the j th layer becomes

$$n_j^2(\omega) = 1 + \frac{f_j}{\omega_j^2 - \omega^2 - i\Gamma_j\omega}, \quad (9)$$

for a characteristic frequency ω_j and a damping coefficient Γ . The other parameter, f_j , is a fraction that denotes the oscillator strength of the material, i.e. we assume a Lorentz profile. For simplicity, the refractive indices are assumed to have only one singularity each. The results in this section are no longer limited to quarter-wave stacks, but we still assume normal incidence.

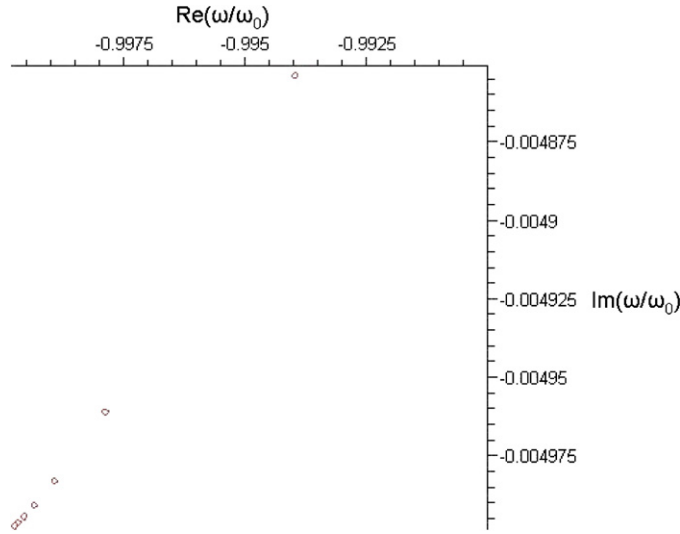


Figure 4. The mode frequencies of a single layer system cluster near the singularities of the refractive index at $(\pm 1, -0.0005)$. The mode frequencies are symmetrical around the imaginary axis. This graph is in units ω_0 .

We will first deal with the case of a single layer system. For the calculation we use the scale of the characteristic frequency, in other words $\omega_j = 1$. Because of (7b) we know that for values of the frequency close to the singularities $\omega = \pm\sqrt{\omega_j^2 - i\Gamma_j\omega}$, which means that $|n_1(\omega)| \gg 1$, the frequencies have to satisfy the following equation:

$$\sin\left(\frac{\omega}{c} \cdot d \sqrt{\frac{f_j}{1 - \omega^2 - i\Gamma_j\omega}}\right) = 0. \quad (10)$$

The other choices for the calculation are: $d = 1$, $f_j = 0.25$, $\Gamma_j = 10^{-3}$ and $n_0 = n_2 = 1$. (The environment of the medium is air or vacuum.) Formula (10) can be derived by setting $m = 2$ in Wolter's recursive formula (5), and neglecting 1 with respect to $\frac{f_j}{\omega_j^2 - \omega^2 - i\Gamma_j\omega}$ because we are near either one of the singularities of (9).

As figure 4 shows, the mode frequencies cluster near the singularities of $n_1(\omega)$. Also, there are no frequencies to the outside of the outermost singularities.

Analogously, for a system of two layers the mode frequencies display the same pattern: near the singularity of the refractive index of each of the respective layers they cluster near the aforementioned singularity. Also, in both cases, there are no mode frequencies to either the left or the right of the outermost singularities of the refractive indices, i.e. no eigenfrequencies with $|\text{Re}(\omega)| \geq \omega_1$. Inserting $m = 3$ into Wolter's recursive formula yields the following transcendental equation for the eigenfrequencies:

$$\begin{aligned} &(1 + g_2)\{(g_2 + g_1)(1 + g_1)\exp(-i\delta_1) - (g_2 - g_1)(g_1 - 1)\exp(i\delta_1)\}\exp(-i\delta_2) \\ &\quad + (1 - g_2)\{(g_2 - g_1)(g_1 + 1)\exp(-i\delta_1) \\ &\quad + (g_2 + g_1)(g_1 - 1)\exp(i\delta_1)\}\exp(i\delta_2) = 0, \end{aligned} \quad (11)$$

where $g_{1,2} = n_{1,2}(\omega)$, $\delta_{1,2} = \frac{\omega}{c}n_{1,2}(\omega)d_{1,2}$ and $g_0 = 1 = g_3$. Now let us look for eigenfrequencies near the resonance of the refractive index of the first layer. This means

that $|g_1| \gg 1$, $|g_1| \gg g_2$, g_2 and $n_2(\omega)$ are approximately constant, and $|\delta_1| \gg 1$, hence we obtain

$$-(1 + n_2(\omega)) \sin\left(\frac{\omega}{c} n_1(\omega) d_1\right) \exp\left(i \frac{\omega}{c} n_2(\omega) d_2\right) + (1 - n_2(\omega)) \sin\left(\frac{\omega}{c} n_1(\omega) d_1\right) \exp\left(-i \frac{\omega}{c} n_2(\omega) d_2\right) = 0. \quad (12)$$

Note that, in principle $n_2(\omega)$ is also frequency dependent, but this can be neglected near the resonance of $n_1(\omega)$. After some manipulations of trigonometric functions we conclude that, instead of (10), the mode frequencies now have to satisfy

$$\sin\left(n_1(\omega) d_1 \frac{\omega}{c}\right) \cos\left(n_2(\omega) d_2 \frac{\omega}{c}\right) + n_2(\omega) \cos\left(n_1(\omega) d_1 \frac{\omega}{c}\right) \sin\left(n_2(\omega) d_2 \frac{\omega}{c}\right) = 0 \quad (13)$$

near the singularity of the first layer (where $n_1(\omega) \gg 1$). The equation for the natural mode eigenfrequencies is

$$\sin\left(n_2(\omega) d_2 \frac{\omega}{c}\right) = 0 \quad (14)$$

near the resonance of the second layer (where $n_2(\omega) \gg 1$). This formula is derived in approximately the same way as (10): the indices of refraction $n_{1,2}(\omega)$ as a function of the frequency are given by equation (9), and neglect 1 with respect to g_2 in equation (11). Equation (14) is the same as (10), so the pattern of the mode frequencies must be the same as well. Near the electron resonance frequency of the first layer ω_1 we see the same clustering accordance with formula (13).

With the aid of a famous theorem from function theory, namely the great Picard theorem it can be shown that such clusterings always occur in a system with an arbitrary number of layers. The great Picard theorem states that an analytic function assumes every complex value, with one possible exception, infinitely many times near an essential singularity². From Wolter's recursive relation (5) it can be concluded that the functions occurring in systems like this are exponential functions (or sines and cosines, if you prefer). In the case of TE polarization, the dispersion model (9) gives rise to singularities both inside and outside the arguments of the exponential functions, so we have an equation of the type $\sum_p A_p(\omega) \exp(i B_p(\omega) \frac{\omega}{c} d) = 0$, where both $A_p(\omega)$ and $B_p(\omega)$ are meromorphic functions of ω with singularities in the complex ω -plane. Only the singularities of the arguments of the exponential functions (those of $B_p(\omega)$) are essential ones, the others are poles. After all, $A_p(\omega)$ is a polynomial in the refractive indices $n_j(\omega)$ which depend on frequency according to (9), and $B_p(\omega)$ depends linearly on $n_j(\omega)$. According to the great Picard theorem, clusterings like those we have seen in two special cases also occur more generally, in any stratified N -layer medium in the case of TE polarization.

If the polarization is transversal magnetic, then the definition of the coefficients g_m changes according to (8). The coefficients δ_m remain the same as in the transversal electric case. This means that the electron resonance frequencies are also essential singularities in the TM case. Therefore, Picard's great theorem can be applied again and there will be a similar clustering near the resonances.

In terms of transmission spectra, we are not quite sure what this distribution of eigenvalues means. Possibly, because of the positions of the natural mode eigenfrequencies in the complex plane, the peaks may shift slightly closer to the origin and become slightly narrower with respect to the peak at $\pm\omega_0$ and the FWHM of $\frac{1}{2}\Gamma$. However, this is not the reason for

² See appendix A.2.

calculating such eigenfrequencies. We have done these calculations because we suspect such clusterings to represent *a complete set of modes* (see the analysis given in the following two sections).

4. The (over)completeness of the natural modes of dispersive media

4.1. Introduction

This section focuses on the question of how ‘physical’ natural modes are, i.e. whether the modes can represent physical quantities such as wavefunctions of electromagnetic radiation. That is why we look into the *completeness* of the natural modes. So the question is if a solution electromagnetic wave equation subject to the boundary conditions set by the stratified N -layer medium, can be written as a linear combination of the natural mode eigenfunctions.

Starting with a one-dimensional wave equation, Leung *et al* [5] showed that the poles of the Fourier transform of the Green’s function, $\widehat{G}(x, y; \omega)$ correspond to the frequencies of the eigenmodes (which Leung calls quasinormal modes). Alternatively put, the poles of $\widehat{G}(x, y; \omega)$ are the natural mode frequencies. Also it was stated that a physically necessary and sufficient condition for completeness of the modes is

$$\lim_{|\omega| \rightarrow \infty} \widehat{G}(x, y; \omega) = 0 \quad (15)$$

in the lower half-plane of the complex variable ω .

However these results did not seem entirely satisfactory, because the modes are actually *overcomplete*; in other words: a representation of the wavefunction or the Green’s function in terms of an eigenfunction expansion is not unique. To determine ‘the degree of (over)completeness’ Leung *et al* [7] introduced a two component formalism: a vector was introduced with one component equal to the wavefunction and the other equal to the time derivative of the wavefunction. From this it was concluded that the natural modes corresponding to one singularity represented the completeness of the expansion of the wavefunction, and the natural modes of the singularity next to it represented the completeness of the time derivative of the wavefunction.

The results of Leung *et al* [5, 6] apply both to non-dispersive media as well as to *dispersive media*. The goal of this section is to extend the results of [6] in the following sense: Leung *et al* [6] showed that an overcomplete set of natural modes is generated by the singularity at ∞ of the dielectric function for ω , namely $\epsilon = \epsilon_\infty + \frac{c_1}{\omega} + \mathcal{O}\left(\frac{1}{\omega^2}\right)$. We will show that *each* singularity of the dispersive dielectric function in the ω -plane, which physically corresponds to a spectral line, generates an overcomplete set of natural modes!

Dispersion is traditionally phenomenologically introduced by assuming that the refractive index depends on the (time) frequency [21]. Therefore, we have to start in frequency space with the Helmholtz’s equation

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\omega^2}{c^2} n^2(x, \omega) \right) \widehat{\psi}(x, \omega) = 0, \quad (16)$$

instead of the usual wave equation (in one dimension). The ‘hatted’ functions denote the temporal Fourier transform of the ‘unhatted’ functions. Furthermore, $n^2(x, \omega)$ is assumed to be a ‘wellbehaving’, differentiable function almost everywhere in the ω -plane and to have a few discontinuities in the x -direction and is supposed to be integrable with respect to x . Note that equation (16) is the 1D Helmholtz equation, which implies we still assume normal incidence.

In order to find out what (16) means to the system in time space we have to apply an inverse Fourier transform

$$\frac{\partial^2}{\partial x^2} \psi(x, t) - \frac{\partial^2}{\partial t^2} \frac{1}{c^2} \int_0^t \rho(x, t - t') \psi(x, t') dt' = 0. \quad (17)$$

The integro-differential equation (17) can be interpreted as a medium with a memory: the whole time interval from zero to t is relevant for the physics and therefore represented in the equation of motion. For instance, in terms of the Lorentz model one can think of electrons that start to oscillate because of the arrival of the em wave. Through these oscillations they affect the part of the wave that has yet to enter the medium. Some books, like [21] introduce dispersion in this way.

4.2. (Over)completeness of the natural modes of a slab

The problem to be addressed to in this section concerns the (over)completeness of the set of natural modes. As we already observed before for the case of a slab each singularity of the refractive index, namely $\omega = \pm\sqrt{\omega_j^2 - i\Gamma_j\omega}$ leads to an infinite number of natural frequencies and natural modes. This statement follows from the observation that close to the singularity the approximate equation to be satisfied by the natural frequencies ω (see (10))

$$\sin\left(\frac{\omega}{c} \cdot d \sqrt{\frac{f_j}{\omega_j^2 - \omega^2 - i\Gamma_j\omega}}\right) = 0, \quad (18)$$

generates for each singularity an infinite number of roots, as the great Picard theorem tells us that near the essential singularities $\pm\sqrt{\omega_j^2 - i\Gamma_j\omega}$ each complex value is obtained an infinite number of times. Hence the question arises whether these successive sets of modes are each complete or not. The key to the solution of this problem is the analysis of the behavior of the distribution of the natural frequencies. We refer to the books by [22] and [23]. Before going into more detail we wish to remark that we will freely switch between the concepts ‘closure’ and ‘completeness’, as Paley and Wiener showed [23] that these two concepts are equivalent (see appendix A.3 for definitions of both terms).

For a slab made of dispersive material, embedded in vacuum, the natural frequencies ω_n are the roots of (7b), and the natural modes read as

$$\sin\left(\frac{\omega_n}{c}x + \phi\right), \quad (19)$$

the natural mode eigenfunctions are therefore specific linear combinations of functions of the form $e^{\pm i\frac{\omega_n}{c}y}$. Paley and Wiener [23] studied completeness properties of this type of functions (see appendix section appendix A.3 for some of their most relevant results).

The goal is now to apply some of the work of Paley and Wiener in order to prove the completeness of systems of natural modes pertaining to a single dispersive slab. More particularly, we wish to apply theorem 7.

We will now apply the Paley–Wiener theorem [23] for the case of a slab and construct therefore the canonical product $F(z)$,

$$F(z) = \prod_{m \neq 0} \left(1 - \frac{z}{\lambda_m}\right) \quad (20)$$

(see (A.16)). The multiplication runs over all the eigenvalues λ_m of a set of natural modes, the zeros of the canonical product must correspond to the eigenfrequencies. Then, the Paley–Wiener theorem tells us that a set of natural modes is then, and only then, complete if the canonical product (20) is *not* square integrable $L^2(\mathbb{R})$.

Alternatively put: furthermore, two cases are distinguished: either the frequency is close to one of the resonances, or its absolute value tends to infinity. In the former case, let

$$z := n(\omega) \Leftrightarrow \lambda_m = n(\omega_m). \quad (21)$$

And if $|\omega| \rightarrow \infty$, then

$$z := \frac{\omega}{c}d \Leftrightarrow \lambda_m = \frac{\omega_m}{c}d. \quad (22)$$

One might say that the canonical product *interpolates* the eigenfrequencies, therefore z is associated with ω and λ_m with ω_m . The reason we distinguish these two cases is that both the resonances and infinity are essential singularities of this system. As we have seen in section 3 such singularities give rise to infinitely many natural modes. Therefore each of these ‘clustering’ is a candidate to be a complete set of modes. (Note that, the fact that there are infinitely many natural modes near one such singularity is not a proof that the modes are complete.) Also it follows from the requirement that the canonical product must be in $L^2(\mathbb{R})$ if and only if it tends to zero faster than $z^{-\frac{1}{2}}$. We shall take advantage of this when investigating the natural modes’ completeness in this section.

We will now show that the canonical product has the following behavior for large values of $|z|$:

$$F(z) = \prod_{m=1}^{\infty} \left(1 - \frac{z}{\lambda_m}\right) \sim p(z) \sin(z), \quad (23)$$

where $p(z)$ is a polynomial in z that may contain negative powers of z

$$p(z) := \sum_{j=-l}^n a_j z^j, \quad l \text{ and } n \text{ are positive integers.} \quad (24)$$

This is the form of the canonical product in both the cases $|\omega| \Rightarrow \infty$ and $\omega \Rightarrow \omega_m$, where ω_m represents the resonance frequency.

First let us consider the case $|\omega| \rightarrow \infty$. According to the dispersion model (9) the refractive index can be approximated by

$$n(\omega) = 1 - \frac{A}{2\omega^2} + O\left(\frac{1}{\omega^3}\right) \quad (25)$$

for a certain constant A . Wolter’s formula (5) for one layer yields the following equation for the eigenfrequencies:

$$\left(2 - \frac{A}{2\omega^2}\right)^2 \exp\left(-i\frac{\omega}{c}\left(1 - \frac{A}{2\omega^2}\right)d\right) - \frac{A^2}{4\omega^4} \exp\left(i\frac{\omega}{c}\left(1 - \frac{A}{2\omega^2}\right)d\right) = 0 \quad (26)$$

multiplying by $\frac{\omega^2}{A}$ gives

$$\sin\left(\frac{1}{i} \log\left(\frac{4\omega^2}{A}\right) + \left(\omega - \frac{A}{2\omega}\right)\frac{d}{c}\right) = 0 \quad (27)$$

which implies that the argument has to equal $m\pi$ (we choose the principal value for the complex logarithm). If $|\omega|$ is chosen sufficiently large, then the term linear in ω will dominate the other terms. Iterating once and neglecting terms of order $\frac{1}{\omega}$ yield

$$\omega_m = \frac{c}{d} \left(m\pi - \frac{1}{i} \log\left(\frac{4m^2\pi^2}{Ad^2}\right) \right) \quad m \in \mathbb{Z} \setminus \{0\}. \quad (28)$$

For this case it seems appropriate to define $z = z'd$, so that $\lambda_m = \frac{\omega_m}{c}d$. From now on we will write z instead of z' . The associated canonical product constructed from the eigenvalues for large values of $|z|$ reads as [23]

$$F(z) = p(z) \prod_{m \in \mathbb{Z} \setminus \{0\}} \left(1 - \frac{z}{m\pi + i \log \left(\frac{4m^2\pi^2}{Ad^2} \right)} \right). \quad (29)$$

It is shown in the appendix that for large values of $|z|$ the modulus of the product $L(z)$

$$L(z) = \prod_{m \in \mathbb{Z} \setminus \{0\}} \left(1 - \frac{z}{m\pi + i \log \left(\frac{4m^2\pi^2}{Ad^2} \right)} \right) \quad (30)$$

tends to a constant. Hence combination of (29) and (30) leads to

$$|F(z)| \sim |p(z)| \cdot \text{const.} \neq 0. \quad (31)$$

Depending on the polynomial $p(z)$ each resonance generates either a (over)complete set of modes if the polynomial contains only positive powers of z , or a set of modes which is not complete if the polynomial contains only negative powers of z . However, if this is the case, such an incomplete set can be made complete by the addition of only a *finite* number of modes generated by one of the other singular points.

This means that for a 1D dispersive stratified N -layer medium, the natural modes are *at least* $N + 1$ -fold complete, if it is assumed that each layer has two resonances. Alternatively put, the Green's function or the wavefunction for a photonic crystal with $2N$ resonances can be expanded in terms of natural mode eigenfunctions in at least $N + 1$ ways.

This completes the proof of (23).

Writing $F(z)$ like equation (23) simply means that we include eigenfrequencies that are still in the vicinity of one of the singularities (either at one of the resonances or at infinity), but not close enough to one of them to display the pattern $\lambda_m = m\pi$.

Equation (A.18) can be verified as follows: let $\epsilon \rightarrow \infty$, $n = 0$ and $A = \epsilon$ then because of the form (23) we can write $F(y + i\epsilon) \sim \exp(\epsilon)$. Also it is clear that condition (A.16) holds: λ_m is at most linear in m . So theorem 7 can be applied.

As the eigenfrequencies ω_m cannot be determined exactly, the precise form of $p(z)$ also remains unknown. The modes that display the pattern $\lambda_m = m\pi$ are *not* complete: they yield $F(z) = \frac{\sin z}{z}$ which is in $L^2(\mathbb{R})$. However, these modes correspond to the case of a clamped string without the important eigenmode $z = 0$ (no oscillation). They do not aptly describe this system as it is open, unlike a clamped string. This does tell us that the modes are not complete if we take the neighborhood around one of the resonances too small. Depending on the asymptotic behavior of $p(z)$, we distinguish two possibilities

- (a) $p(z)$ only contains negative powers of z . As $F(z)$ is an entire function, a sufficient condition for $F(z)$ to be in $L^2(\mathbb{R})$ is

$$\lim_{x \rightarrow \infty} \sqrt{x} F(x) = 0, \quad (32)$$

where x is real. So in this case the canonical product is in $L^2(\mathbb{R})$, and according to theorem 7 the natural modes are not complete. The same theorem also states that in this case, the corresponding set of eigenfunctions can be made complete by the adjunction of a finite number of functions of a similar form. To this end, some other natural mode eigenfunctions can be used. However, there is no physical reason to prefer one natural mode to another. Neither is there a physical reason why, say, q natural modes are required to make them complete and not another number.

- (b) $p(z)$ contains at least one positive power of z . Then $F(z) \notin L^2(\mathbb{R})$ and the natural modes in this area are complete.

Whichever possibility is the correct one, from physical considerations it seems that the natural modes in the neighborhood of the resonances are complete anyway. If more layers are added to the system, more resonances will occur. This means there will also be more clusterings of natural modes near these resonances. So, a system of N slabs is at least N -fold complete, even if $p(z)$ contains only negative powers of z .

5. Conclusions

The analysis of the pertinent properties of these fundamental modes, *to be considered as the most ‘natural’ set of functions for the expansion of the field*, is of paramount interest. The completeness property of the field is especially one of the most important and interesting features of these modes are to be studied. In some special cases, for instance in a non-dispersive, periodic 1D SNL medium with quarter-wave stacks, the natural modes formalism is an efficient tool to reveal information about transmission spectra of such media.

In [5], Leung *et al* showed that, for a system described by the 1D wave equation without dispersion, a sufficient (and possibly necessary) condition for completeness of the natural modes is that the Fourier transformed Green’s function vanishes for sufficiently large frequencies. The generalization to dispersive media is relatively straightforward: the same condition applies, although the expression for eigenmode expansion coefficients is slightly more complicated [6]. This result is obtained without outlining a specific dispersion model.

In order to investigate the degree of (over)completeness of natural modes in 1D photonic crystal we have chosen the following dispersion model:

$$n_j(\omega) = \sqrt{1 + \frac{f_j}{\omega_j^2 - \omega^2 - i\Gamma_j\omega}}$$

for the j th layer of the medium. If each layer of the photonic crystal is assumed to have two resonance frequencies, then the natural modes in a medium of N layers is at least $N + 1$ fold complete. As of yet, we are unsure of what this tells us about either the natural mode formalism or the used dispersion model.

(Over)completeness of the natural mode expansion may imply that natural modes are ‘physical’ in a certain way, but it does not mean that they are useful (we may still need an unpractically large number of modes to aptly describe our system). Based on [24] we suspect that, in the typical photonic crystal region, where the wavelength of the electromagnetic radiation is of the same order of magnitude as the thickness of a layer, that electromagnetic wave couples to only a few modes. Currently, however, there is still no proof of this.

Our results were derived for dispersive SNL media with normal incidence. To generalize to 2D systems (i.e. for $\theta_m \neq 0$ in figure 1) Wolter’s recursive formula (5) can still be used. Obviously the angle of incidence θ_m does not depend on frequency but the angles of refraction do, which would complicate such an analysis. However it seems likely that the Lorentz resonances also form essential singularities in this case, and hence the natural mode frequencies also cluster near the resonances. (The only way for this *not* to happen would be if the frequency dependence of the angles of refraction somehow removed the essential singularities.) So in 2D we would expect the same degree of ‘overcompleteness’ to occur as in 1D. In 3D, Wolter’s formula is no longer valid because both the TM and the TE modes contribute to the electromagnetic pulse. In this case, the transfer matrix method [19] can be used to investigate the completeness properties of the natural modes.

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Appendix A. Mathematical theorems on the properties of functions

A.1. Roots of exponential sums

Equation (5) shows that trying to find the natural mode frequencies leads to a transcendental equation (more specifically, an exponential sum). Mathematicians studied roots of such equations in the 1930s. In this appendix, some useful theorems and results will be given (without proof). For more details see [27], [28] and [29].

Langer [27] derived the following theorem:

Theorem 1. *If the constants B_j are real and*

$$0 = B_0 < B_1 < \cdots < B_J \quad (\text{A.1})$$

then for $|\rho|$ sufficiently large the roots of the equation

$$\sum_{j=0}^J [b_j] e^{\rho B_j} = 0, \quad b_0 \neq 0, \quad b_J \neq 0 \quad (\text{A.2})$$

lie in the strip bounded by the lines

$$\operatorname{Re}(\rho) = \pm c, \quad (\text{A.3})$$

where c is a suitably chosen real constant. The number N of roots lying in any interval of this strip of length l satisfies the relation

$$B_J l / (2\pi) - (J + 1) \leq N \leq B_J l / (2\pi) + (J + 1). \quad (\text{A.4})$$

Moreover if ρ remains uniformly away from the zeros of (A.2) the left-hand member of the equation is uniformly bounded from zero.

This result is useful because it concerns exponential sums of the type we have encountered in sections 2 and 3. Because the imaginary unit i occurs in arguments of the exponents of the sum in (5), the imaginary parts of the natural mode frequencies are bounded. Also theorem 1 tells us that the number of roots is proportional to the length of the strip. This implies that there are infinitely many natural modes in the entire complex plane (if we stay sufficiently far away from the origin).

The next result, which Langer [28] obtained a few years later, is also relevant to us.

Theorem 2. *If in the exponential sum*

$$\Phi(z) = \sum_{j=0}^n A_j e^{c_j z} \quad (\text{A.5})$$

the coefficients are constant and the exponents commensurable (the arguments of the exponents are integer multiples of each other), the sum becomes of the form

$$\Phi(z) = \sum_{j=0}^n a_j (e^{\alpha z})^{p_j}, \quad p_0 = 0, \quad p_j \in \mathbb{N} \quad (\text{A.6})$$

and the distribution of the zeros is given explicitly by the formula

$$z = \frac{1}{\alpha} (2m\pi i + \log \xi_j), \quad \xi_j := e^{\alpha z} \quad (\text{A.7})$$

where $m \in \mathbb{Z}$ and j is a natural number $\leq p_n$.

This may seem complicated at first but the special case of commensurable exponents is actually theoretically the simplest one, because it makes the problem of the distribution of the zeros essentially an algebraic one. This is also the theorem we used for the calculations in sections 2 and 3. The assumption of commensurability is no doubt a limiting one, but it includes a few important special cases, such as a trigonometric sum (a partial sum of a Fourier series).

Also, without assuming commensurability, Langer [28] showed that theorem 1 is not only valid far away from the origin, but everywhere in the complex plane.

A.2. Some theorems from function theory

Theorem 3 ('Great Picard Theorem'). *Suppose an analytic function $f(z)$ has an essential singularity at $z = a$. Then in each neighborhood of a , $f(z)$ assumes each complex value, with one possible exception, an infinite number of times.*

Proof and corollaries can be found in most textbooks on function theory, like [30].

This is the type of singularity we encountered in section 3. The analytic function in this case is the denominator of the reflection coefficient. The essential singularity is the (electron) resonance frequency. Of course zero includes the complex values this function assumes infinitely many times near the essential singularity, which explains the clustering of roots displayed in figure 2.

The 'one possible exception' is any function of the form $e^{1/z}$ near $z = 0$. This type of function cannot assume zero since it has no roots.

We also require the

Theorem 4 ('Weierstrass factorization theorem'). *Let f be an entire function and let $\{a_n\}$ be the nonzero zeros of f repeated according to multiplicity; suppose f has a zero of order $m \geq 0$ (a zero of order 0 at $z = 0$ means $f(0) \neq 0$). Then there is an entire function g and a sequence of integers $\{p_n\}$ such that*

$$f(z) = z^m e^{g(z)} \prod_{n=1}^{\infty} E_{p_n}\left(\frac{z}{a_n}\right), \quad (\text{A.8})$$

where for every natural number p

$$\begin{aligned} E_0(z) &:= 1 - z \\ E_p(z) &:= (1 - z) \exp\left(z + \frac{z^2}{2} + \cdots + \frac{z^p}{p}\right), \quad p \geq 0. \end{aligned} \quad (\text{A.9})$$

The numbers p_n are chosen in such a way that the series

$$\sum_n \left(\frac{z}{|a_n|}\right)^{1+p_n} < \infty. \quad (\text{A.10})$$

The function $E_p(z)$ is known as the *elementary factor*. Note that $E_p(\frac{z}{a})$ has a simple root at $z = a$ no other roots. In a way this is a generalization of Gauss' main theorem of algebra about the factorization of polynomials.

A.3. Equivalence of closure and completeness in L^2_{loc}

The set of functions $\{f_n(x)\} \subset L^2(a, b)$ ($a, b \in \mathbb{R}, a > b$) is said to be *closed over* (a, b) if

$$\int_a^b f(x) f_n(x) = 0 \quad (\text{A.11})$$

implies $f(x) \equiv 0$ almost everywhere on (a, b) $\forall f(x) \in L^2(a, b)$. The set of functions $\{f_n(x)\}$ is said to be *complete* if $\forall f(x) \in L^2(a, b), \varepsilon > 0$ there is a polynomial

$$P_n(x) = \sum_{k=1}^n a_k f_k(x) \quad (\text{A.12})$$

such that

$$\int_a^b |P_n(x) - f(x)|^2 < \varepsilon. \quad (\text{A.13})$$

For all practical intents and purposes, we can think of this as $P_n(x) = f(x)$, because in our application $f(x)$ is a solution of a differential equation, so this more general formulation is not needed for it. In [23] Paley and Wiener proved that

Theorem 5. *A set of functions $\{f_n(x)\} \subset L^2(a, b)$ is closed over (a, b) if and only if it is complete.*

This theorem is not hard to intuitively picture: it states that the only square integrable function that is orthogonal to all functions of a complete set is the function that is identical to zero. Analogously we can imagine that the only vector perpendicular to all the vectors of a complete set of vectors is the vector with length zero.

We will need this relationship between closure and completeness for theorem 7. Also it will be assumed that

$$\lim_{n \rightarrow \infty} \frac{\lambda_n}{n} = 1. \quad (\text{A.14})$$

In this case the entire function

$$F(z) = \prod_{n=1}^{\infty} \left(1 - \frac{z^2}{\pi^2 \lambda_n^2}\right) \quad (\text{A.15})$$

exists according to theorem 4. (This statement follows from the conditions for this theorem 4, taking $p_n = 0$.)

Theorem 6. *Let (A.14) be true. Furthermore, let $F(z) \in L^2(\mathbb{R})$. Then the set of functions $\{e^{\pm i\lambda_n x}\}$ cannot be closed over (a, b) . Again, let $zF(z) \in L^2(\mathbb{R})$. Then the set of functions $\{1, e^{\pm i\lambda_n x}\}$ cannot be closed on $L^2(a, b)$. In either case, a finite number of the functions of the set may be replaced by an equal number of other functions of the form $e^{i\lambda x}$.*

For this application main theorem on the completeness (closure) of sets of functions of the exponential type [23] is given below

Theorem 7. *Let*

$$\lim_{m \rightarrow \infty} \frac{|\lambda_m|}{m} = 1 \quad (\text{A.16})$$

then according to the Weierstrass factorization theorem (see theorem 4 in appendix A.2 from appendix A) the following entire function exists:

$$F(z) = \prod_{m=1}^{\infty} \left(1 - \frac{z^2}{\pi^2 \lambda_m^2}\right) \quad (\text{A.17})$$

and let

$$|F(y + i\epsilon)| \geq \frac{A}{1 + |y|^n} > 0 \quad (\text{A.18})$$

for all real y , some $A > 0$, and some ϵ and n . Then the set of functions $\{e^{\pm i\lambda_m y}\}$ will be closed or not closed on $L^2(a, b)$ according to the fact that $F(z)$ does not or does belong to $L^2(\mathbb{R})$. It can always be made closed by the adjunction of a finite number of functions $e^{i\lambda y}$. The set of functions $\{1, e^{\pm i\lambda_m y}\}$ will be closed or not closed on $L^2(\mathbb{R})$ according to the fact that $zF(z)$ does or does not belong to $L^2(\mathbb{R})$.

Another relevant result by Paley and Wiener is the following:

Theorem 8. Let (A.14) be true and let the set of functions $\{e^{\pm i\lambda_n x}\}$ be closed on $L^2(a, b)$ but let it cease to be closed on the removal of some one term. Then it ceases to be closed on the removal of any one term, $F(z) \notin L^2(\mathbb{R})$, but $F(z) \in L^2(1, \infty)$. Again, if the set of functions $\{1, e^{\pm i\lambda_n x}\}$ is closed on $L^2(a, b)$, but ceases to be closed on the removal of some one term, this term is arbitrary, then $zF(z) \notin L^2(\mathbb{R})$ but $F(z) \in L^2(\mathbb{R})$.

Appendix B. The derivation of (31)

We start from the product $L(z)$

$$L(z) = \prod_{m \in \mathbb{Z} \setminus \{0\}} \left(1 - \frac{z}{m\pi + i \log \left(\frac{4m^2\pi^2}{Ad^2} \right)} \right). \quad (\text{B.1})$$

Taking the logarithm of both the left-hand side and the right-hand side of equation (29) yields

$$\log(L(z)) \sim P \int_{-\infty}^{\infty} \log \left(1 - \frac{z}{m\pi + i \log \left(\frac{4m^2\pi^2}{Ad^2} \right)} \right) dm, \quad (\text{B.2})$$

where P denotes the Cauchy principal value. The ‘ \sim ’ changes into an equal sign if the steps in the canonical product are small enough. Then $\log(L(z))$ becomes a Riemann sum of the integral occurring on the right-hand side of (B.2).

Integration by parts changes the integrand into a fraction

$$P \int_{-\infty}^{\infty} \frac{mz(\pi + i \frac{2\pi^2}{Ad^2 m}) dm}{[m\pi + i \log \left(\frac{m^2\pi^2}{Ad^2} \right)]^2 + z(m\pi + i \log \left(\frac{m^2\pi^2}{Ad^2} \right))}. \quad (\text{B.3})$$

Substituting $p_m := m\pi + i \log \left(\frac{m^2\pi^2}{Ad^2} \right)$ simplifies this integral considerably

$$\log(L(z)) \sim P \int_{-\infty}^{\infty} \frac{m \frac{dp_m}{dm} z dm}{p_m(p_m + z)}. \quad (\text{B.4})$$

The integrand has two poles that correspond to $p_m = -z$

$$m'_{\pm}(z) := \frac{2i}{\pi} W \left(\pm \frac{i}{2} d\sqrt{A} \exp \left(\frac{iz}{2} \right) \right), \quad (\text{B.5})$$

and two poles at $p_m = 0$

$$m'_{\pm}(z = 0) = W \left(\pm \frac{i}{2} d\sqrt{A} \right), \quad (\text{B.6})$$

where W denotes the (principal value of the) *Lambert W-function* [25, 26]. This function is defined as the multi-valued solution $W(z)$ of the equation $z = W(z) \exp(W(z))$. The principal value solution is one of the two real branches. As we chose the principal value of the complex

logarithm, we also find the poles in terms of the principal value of the Lambert W -function. The residues near these poles are

$$-\frac{2i}{\pi}(m_+(z) + m_-(z) + m_+(z=0) + m_-(z=0)) - \frac{4i\pi^2}{Ad^2}. \quad (\text{B.7})$$

The terms with $m_{\pm}(z=0)$ correspond to the contribution due to the two poles at $p_m = 0$. Multiplying this by $2\pi i$ yields the outcome of the integral. Because we have chosen the principal value of $\log(L(z))$ we wish to estimate the modulus of this outcome. In order to do so we use the relation $|W(z)| = W(|z|)$

$$0 < \left| \frac{8}{\pi}(m_+(z) + m_+(z=0)) + \frac{8\pi^3}{Ad^2} \right| \leq \frac{16}{\pi} W\left(\frac{1}{2}\sqrt{Ad}\right) + \frac{8\pi^3}{Ad^2} \quad (\text{B.8})$$

which does not depend on z ! So the absolute value of the product (B.1) behaves as

$$|L(z)| \sim \text{const.} \neq 0. \quad (\text{B.9})$$

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